ABSTRACT

Predictive modeling is an important part of evaluating natural attenuation for groundwater contaminant plume remediation. This paper presents a numerical groundwater contaminant fate and transport model that was developed within a spreadsheet program for this purpose. The model accounts for site heterogeneity and multiple degradation regions, offering flexibility and ease of application. A two-dimensional finite-difference approach integrated with a fourth-order Runge-Kutta method for numerical solution was used as the mathematical foundation. The model was used to evaluate natural attenuation for removal of a trichloroethylene (TCE) plume from a surficial aquifer containing three regions with distinctly different processes for degradation of TCE. Model simulations were used to predict how far the TCE plume would migrate within the aquifer. Based on model results natural attenuation was judged to be sufficient to prevent migration to a potential receptor of the TCE plume.

KEYWORDS: natural attenuation, numerical modeling, spreadsheet, finite-difference, Runge-Kutta

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TROY MATTHEW TWESME

and have found that it is complete and satisfactory in all respects,
and that any and all revision required by the final
examining committee have been made.

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Signature of Faculty of Advisor

August 18, 1999

Date

GRADUATE SCHOOL

NUMERICAL SPREADSHEET MODELING OF NATURAL ATTENUATION FOR GROUNDWATER CONTAMINANT PLUMES

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Overview

Evaluation of natural attenuation as a remedial alternative for groundwater contaminant plumes is accomplished with fate and transport models. Numerical models for this purpose can easily be developed within spreadsheet programs that are available on most personal computers. These programs offer an easy to use template for development of numerical models that are capable of incorporating site heterogeneities and multiple contaminant loss mechanisms.

The following paper has been submitted for publication in *Ground Water Monitoring and Remediation.* The paper describes the development and application of a two-dimensional numerical contaminant fate and transport model that was formulated in a spreadsheet program. The model was specifically developed for application to the Trio Solvents site in New Brighton, MN, where a heterogeneous surficial aquifer is contaminated by Trichloroethylene (TCE).

Alliant Technologies, Inc. is the responsible party for the site and provided funding for the natural attenuation study. Conestoga-Rovers and Associates is the consulting firm tasked with managing the remediation efforts at the site. After five years of groundwater extraction efforts (1991-1996) failed to eliminate the contamination, regulators allowed the extraction pumps to be turned off so the University of Minnesota could conduct a natural attenuation study. As an add-on to the natural attenuation study, this modeling effort was conducted in order to offer a prediction on the fate of the TCE plume.

NUMERICAL SPREADSHEET MODELING OF NATURAL ATTENUATION FOR GROUNDWATER CONTAMINANT PLUMES

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ABSTRACT

Predictive modeling is an important part of evaluating natural attenuation for groundwater contaminant plume remediation. This paper presents a numerical groundwater contaminant fate and transport model that was developed within a spreadsheet program for this purpose. The model accounts for site heterogeneity and multiple degradation regions, offering flexibility and ease of application. A two-dimensional finite-difference approach integrated with a fourth-order Runge-Kutta method for numerical solution was used as the mathematical foundation. The model was used to evaluate natural attenuation for removal of a trichloroethylene (TCE) plume from a surficial aquifer containing three regions with distinctly different processes for degradation of TCE. Model simulations were used to predict how far the TCE plume would migrate within the aquifer. Based on model results natural attenuation was judged to be sufficient to prevent migration to a potential receptor of the TCE plume.

KEYWORDS: natural attenuation, numerical modeling, spreadsheet, finite-difference, Runge-Kutta

Introduction

Natural attenuation is recognized as a viable means for remediating contaminated groundwater (U.S. Environmental Protection Agency, 1997). The processes that constitute natural attenuation include dispersion, adsorption, biodegradation, chemical reactions, and/or radioactive decay (Suthersan, 1997). Although these processes occur at most contaminated sites, they may be environmentally significant at only some (Brady et al., 1998). Thus, natural attenuation must be evaluated for effectiveness before it can be considered as a remedial option.

An appropriate evaluation involves the documentation of actual contaminant loss at the site, as well as laboratory studies in which the mode(s) of attenuation are identified (Wiedemeier T.H. et al., 1996). If the data indicate that natural attenuation is a feasible remedial alternative, then models for contaminant transport and removal are necessary in order to predict the *in situ* contaminant fate (Brady et al., 1998). The predictions can then be used to evaluate the timeliness of the process and the potential for transport of contaminants to downgradient receptors.

Many of the models currently used for making these predictions are limited to homogeneous sites, including several that are based on the finite-difference method which is generally accepted as the simplest and most intuitive (Bear and Verruijt, 1987). However, most sites are not homogeneous, with considerable variation in the parameters that affect transport and degradation. Models based on the finite-difference method can take these heterogeneities into account by a descritization process that produces an array of coupled domains; each domain is treated as homogenous with its own parameters for

transport and degradation. Taken together, the individual domains yield a migration profile of the contaminant plume.

This study describes the development and application of a two-dimensional (2-D) finite-difference spreadsheet model used to evaluate natural attenuation of groundwater contaminant plumes at heterogeneous sites. The model was applied to a field site where a trichloroethylene (TCE) plume is migrating through a shallow unconfined aquifer and wetland system towards a freshwater lake.

Model Theory and Background

In saturated porous media, contaminants are subject to advective and dispersive transport as well as sorption, desorption and removal by degradation. For two-dimensional transport, the general equation used to describe these influences when subjected to unidirectional flow is

$$\frac{\partial C}{\partial t} = \frac{D_x}{R}\frac{\partial^2 C}{\partial x^2} + \frac{D_z}{R}\frac{\partial^2 C}{\partial z^2} - \frac{v_x}{R}\frac{\partial C}{\partial x} - kC \qquad (1)$$

where C = concentration of solute in liquid phase (ML^{-3}); t is time; v_x = average linear groundwater velocity (LT^{-1}); D_x and D_z are longitudinal and transverse hydrodynamic dispersion coefficients (L^2T^{-1}); R = retardation factor; k = first order reaction constant (T^{-1}) (Javandel et al., 1984). Horizontal and vertical distances are designated by x and z, respectively. In the unit designations M = mass, L = length, and T = time.

The retardation factor (R) within Equation 1 accounts for the sorption and desorption of solutes to aquifer sediment; for aliphatic hydrocarbons such as TCE R can be described (Chiou et al., 1979) by the linear relationship

$$R = 1 + \frac{\rho_b K_d}{\theta} \quad (2)$$

where K_d = equilibrium distribution coefficient (L^3M^{-1}), ρ_b = dry bulk mass density of the sediment (ML^{-3}); and θ = porosity of the porous medium (Fetter, 1993).

In fate and transport models a finite-difference form of Equation 1, obtained by substituting algebraic differences for each partial derivative, is often used to approximate the solution (Bear & Verruijt, 1987). In this form Equation 1 is

$$\frac{\Delta C_i}{\Delta t} = \frac{D_x}{R}\frac{(C_{i+1,j} - 2C_{i,j} + C_{i-1,j})}{\Delta x^2} + \frac{D_Z}{R}\frac{(C_{i,j+1} - 2C_{i,j} + C_{i,j-1})}{\Delta z^2} - \frac{v_x}{R}\frac{(C_{i,j} - C_{i+1,j})}{\Delta x} - kC \quad (3)$$

where Δt = length of time-step; Δx = length of segment in x direction; Δz = length of segment in z direction. Subscripts i and j count cells in the x- and z-directions, respectively.

When using Equation 3 the subsurface region (model domain) is divided into a grid of discrete segments that can account for site heterogeneity. After contaminant concentrations along the domain boundary and within each segment at the beginning of the computation (initial condition) are established, Equation 3 is used to calculate the change in concentration within each segment over time. The model domain and corresponding equations can easily be represented within computer spreadsheets, with each segment of the domain depicted by a spreadsheet cell. Separate sheets are designated for the transport and degradation parameters and each sheet has a sole parameter value for each segment. The manual iteration feature of the spreadsheet program can be used to calculate the change in concentration within a cell after each time-step based on concentrations calculated in the previous time-step.

The discretization process used in the finite difference method induces numerical dispersion similar to physical dispersion (Bajracharya and Barry, 1994). The Peclet number and Courant number are dimensionless ratios that are used as criteria for finding the optimal segment and time-step length in order to limit numerical dispersion and maintain model stability (Rao and Hathaway, 1989). The Peclet number (Pe), a ratio of the advective to diffusive terms in the transport equation, is defined as

$$Pe = \frac{v_x \Delta x}{D_x} \tag{4}$$

The Courant number (Co) is the ratio of the advective to time dependent terms in the transport equation and is defined as

$$Co = \frac{v_x \Delta t}{\Delta x} \tag{5}$$

Generally, numerical dispersion is minimized and model stability maximized by maintaining a Peclet number less than or equal to two and a Courant number less than or equal to unity (Pinder and Gray, 1977). If these criteria are met, the finite difference model can nearly result in the same solutions for Equation 1 as analytical (exact) solutions. If the Peclet or Courant numbers are larger than the criteria, model results must be closely scrutinized.

We eliminated the need to iterate to a specific convergence criterion in each time step and improved the accuracy of the model's approximations by solving Equation 3 in each segment by a fourth-order Runge-Kutta method. The fourth-order Runge-Kutta method was applied in the form

$$C_{i+1} = C_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$
$$k_1 = hf(C_i)$$
$$k_2 = hf(C_i + \frac{1}{2}k_1) \quad (4)$$
$$k_3 = hf(C_i + \frac{1}{2}k_2)$$
$$k_4 = hf(C_i + k_3)$$

where h = length of time-step and $f(C_i)$ is the derivative given by the right-hand side of Equation 3 (Zill, 1997).

Model Verification

Output from the spreadsheet model was compared to analytical solutions to establish model accuracy and to verify that the basic equations were being solved correctly. Analytical solutions given by Javandel et al. (1984) for two-dimensional contaminant transport in porous media with one-dimensional uniform flow were used for the comparison. The example consisted of a unidirectional flow system with a continuous conservative contaminant source (Figure 1) and normalized transport parameters that are dominated by longitudinal dispersion.

Spreadsheet model simulations were run for four cases (Table 1). All four cases closely matched the analytical solutions given by Javandel et al. (Figures 2 and 3). Cases 1 and 2 provided the best fit in the longitudinal direction because of the smaller longitudinal segment length. Cases 1 and 3 provided the best fit in the transverse direction due to the smaller transverse segment length. Case 4 seemed to suffer an increase in numerical dispersion in both directions. A simulation using the conditions listed for Case 1, except that Δt was set equal to 0.1 day (Co = 0.005), was also

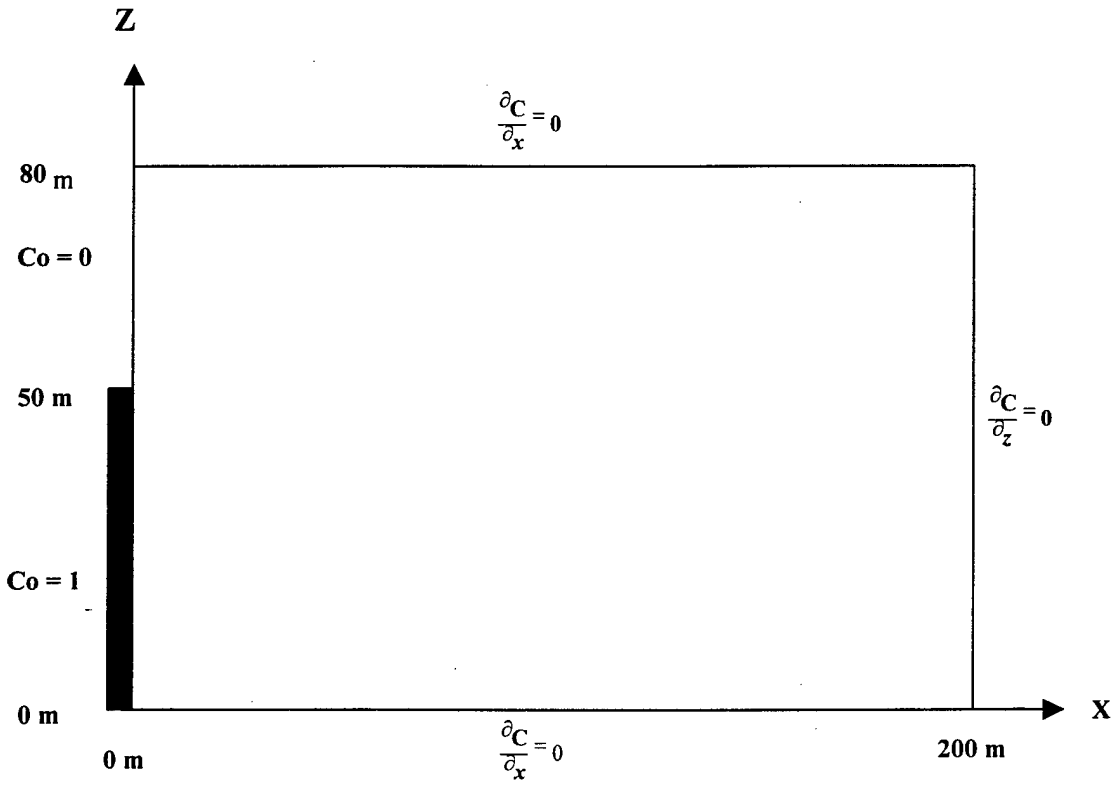

Figure 1: Rectangular flow domain with continuous source and zero flux boundaries for model verification simulations.

Table 1: Discretization and Transport Parameters for Verification Problem

Case	Pe	Co	Δx (m)	Δy (m)	Δt	Vx (md^{-1})	Dx (m^2d^{-1})	Dz (m^2d^{-1})
1	0.2	0.05	2	2	1	0.1	1	0.1
2	0.2	0.05	2	5	1	0.1	1	0.1
3	0.5	0.02	5	2	1	0.1	1	0.1
4	0.5	0.02	5	5	1	0.1	1	0.1

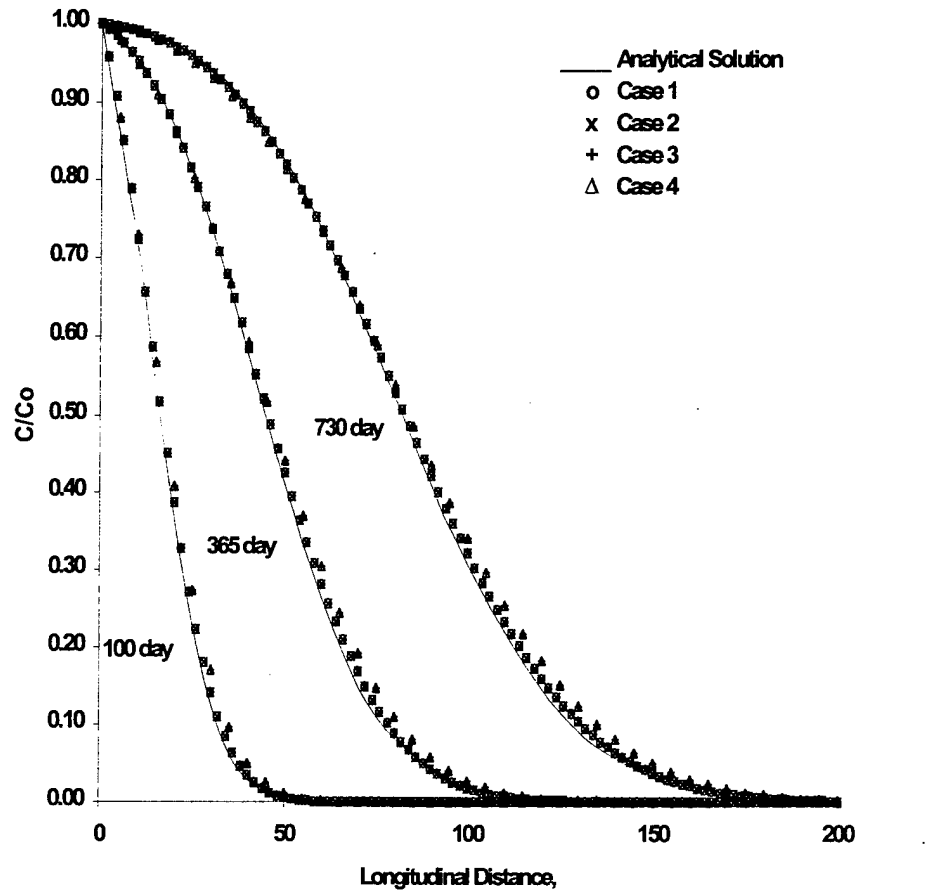

Figure 2: Comparison of four cases of spreadsheet model output to analytical solutions adapted from Javandel et al. (1984) for the flow domain defined in Figure 1. Longitudinal concentration profiles along the x-axis from model simulations.

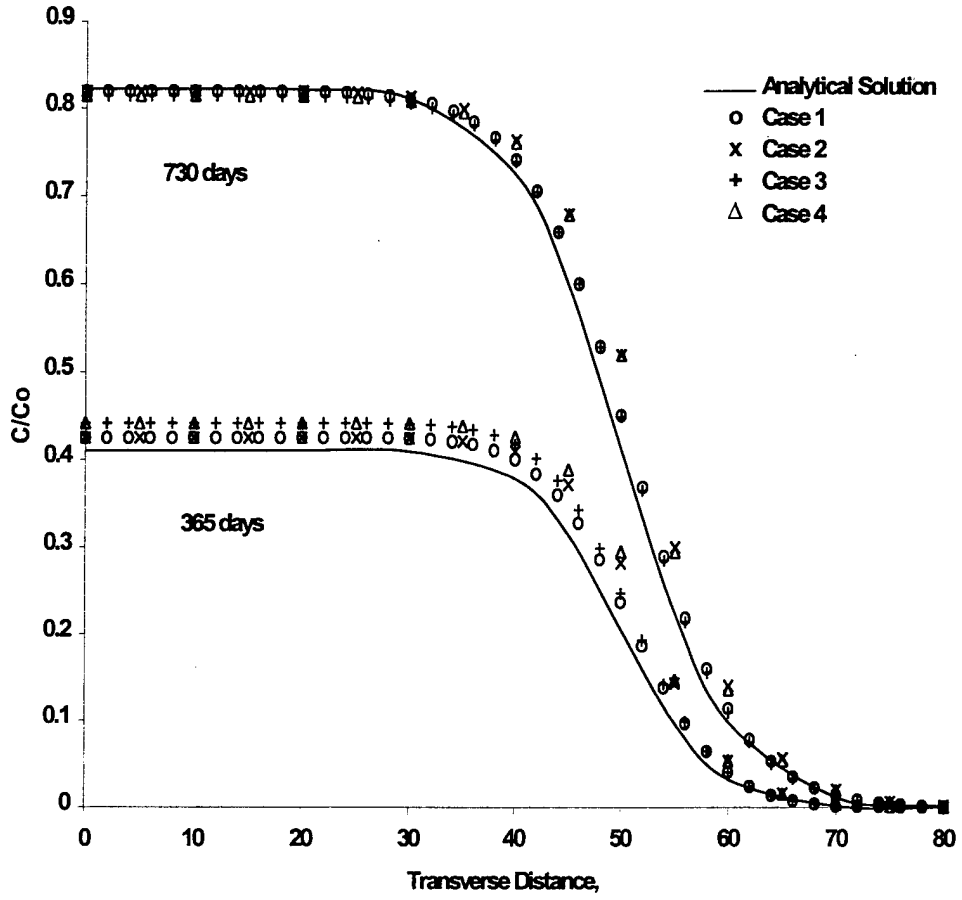

Figure 3: Comparison of four cases of spreadsheet model output to analytical solutions adapted from Javandel et al. (1984) for the model domain defined in Figure 1. Transverse profiles along the z-axis at x = 50 m from model simulations.

completed (results not shown). Results did not vary noticeably from results with $\Delta t = 1$. However, in simulations completed with the Courant number greater than 0.2, the model became unstable.

Modeling of a dispersion-dominated problem while satisfying the Peclet criterion was easy, however if the example was advection-dominated (i.e. $v_x = 1$ md^{-1} and $D_x = 0.1$ m^{2}d^{-1}) the spatial step size needed to be less than or equal to 0.2 m in order to meet the criterion. This results in a model domain consisting of at least 1000 segments along the longitudinal flow direction as compared to 10 or more segments in the dispersion dominated example. Such an increased number of segments increases model simulation time.

Model Application to the Trio Solvents Field Site

The model was applied to a former solvent distillery site in New Brighton, Minnesota where a surficial aquifer is contaminated with trichloroethylene. A groundwater extraction system was in operation from 1991-1996 removing approximately 70 kg of TCE, but the system was shut down after initial average groundwater TCE concentrations of 2200 ppb leveled off near 200 ppb. Two years later, the average TCE concentration in the groundwater was 300 ppb. The plume of residual TCE is migrating northeast from the source area impacting a stand of cottonwood trees and then a wetland that is connected to a freshwater lake (Figure 4).

The surficial aquifer is composed of fine to medium grained sand and silty sand with a depth of approximately 10 m and a water table varying between 0 to 1 m below the land surface (Delta, 1987; Conestoga-Rovers and Associates, 1990). TCE transformation

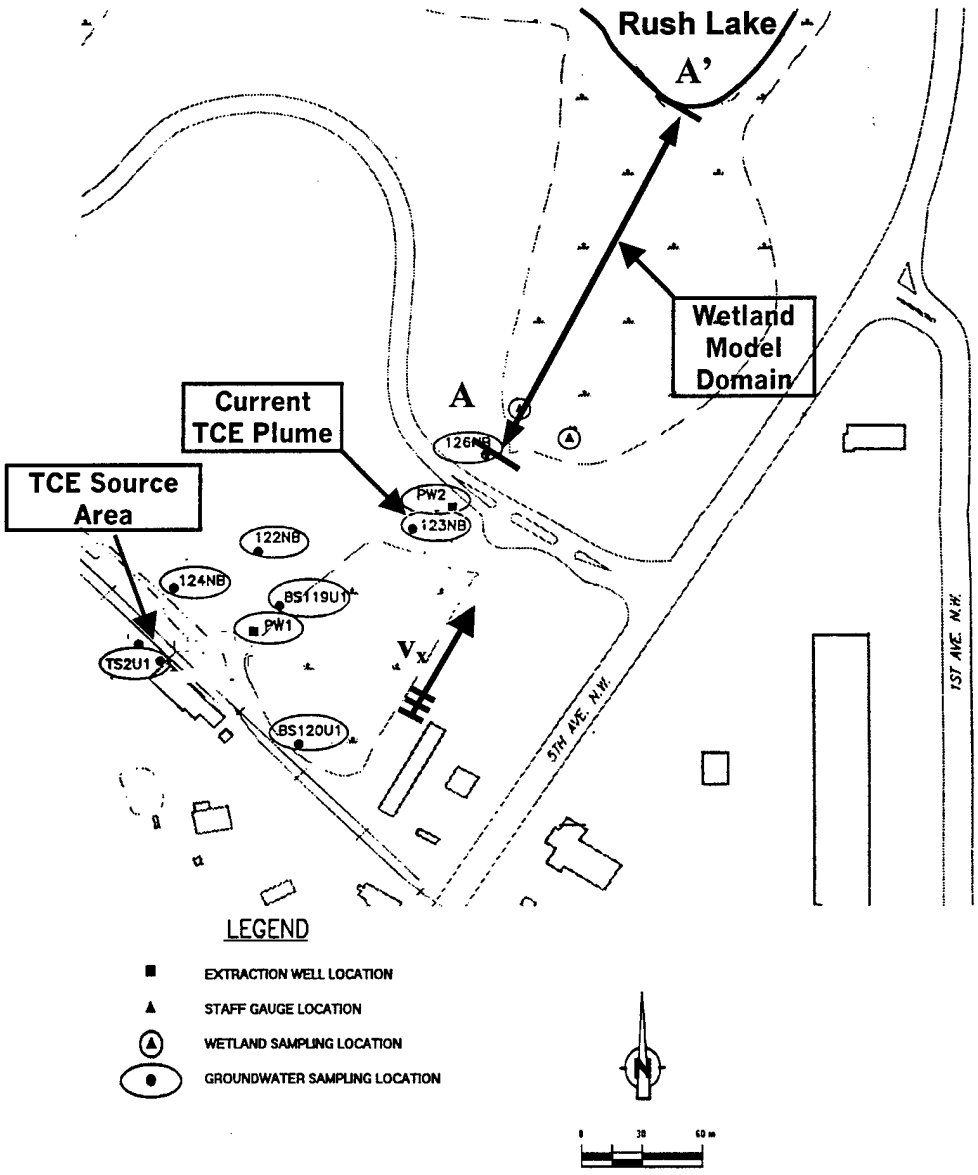

Figure 4: Aerial View of Trio Solvents Site showing TCE Source Area, Groundwater Flow Direction, and Model Domain (A to A'). (Adapted from Conestoga-Rovers and Associates, 1990).

products are present in the groundwater (*cis*-1,2-dichloroethylene and vinyl chloride) and laboratory studies showed evidence of TCE removal by indigenous processes (Bankston et al. 1999), indicating that site conditions are favorable for natural attenuation.

The actual amount of TCE spilled in the past is unknown, so determination of current source amounts was impossible. Therefore a continuous source of TCE using concentration profiles obtained from groundwater measurements collected over the last two years (Bankston et al. 1999) was used as input to the model domain.

The model domain was defined as the area between the observed leading edge of the plume and Rush Lake (A to A' in Figure 4). Bankston (1998) identified three regions within this domain having distinctly different processes for the degradation of TCE. A clay lens about 4 m below the surface was also identified. Table 2 gives a summary of the estimated ranges for transport and degradation parameters and Figure 5 gives the vertical configuration of the aquifer assumed for the model domain.

Prior to running the 2-D simulations for the entire domain, one-dimensional simulations of a TCE concentration profile from A to 100 m downgradient were run for a 6500 day period and three different segment lengths in order to investigate how Peclet numbers affected model output (Figure 6). A simulation that used a segment length of 0.012 m to meet $Pe < 2$ criterion was not run, because the number of segments needed to represent the domain exceeded available desktop computer memory capabilities. However, other models have yielded good results with Peclet numbers as high as ten (Elnawawy & Valocchi, 1990). Therefore a simulation with a segment length of 0.028 m ($Pe = 5$) was run, requiring over 3500 segments to discretize the domain. A reduction in time-step length to 1/10 of a day ($Co = 0.15$) was necessary in order to maintain model

Table 2: Range Estimates for Transport and Degradation Parameters

Parameter	Low Estimate	Mid-Range	High Estimate	Reference
Groundwater velocity (md^{-1})	8.3×10^{-3}	4.2×10^{-2}	9.1×10^{-2}	Delta (1987) CRA (1990)
Longitudinal dispersion (m^2d^{-1})	2.3×10^{-5}	1.2×10^{-4}	1×10^{-3}	Bear (1979)
Transverse dispersion (m^2d^{-1})	6.3×10^{-6}	1.3×10^{-5}	9.4×10^{-5}	Bear (1979)
Aquifer sediment decay constant (day^{-1})	.00042[b]	.0077	.04[a]	a-Appendix B b-Howard et al. (1991)
Cottonwood tree decay constant (day^{-1})	.00305	.0305	.305	Bankston et al. (1999)
Cattail and wetland sediment decay constant (day^{-1})	.00234	.0234	.234	Bankston et al. (1999)

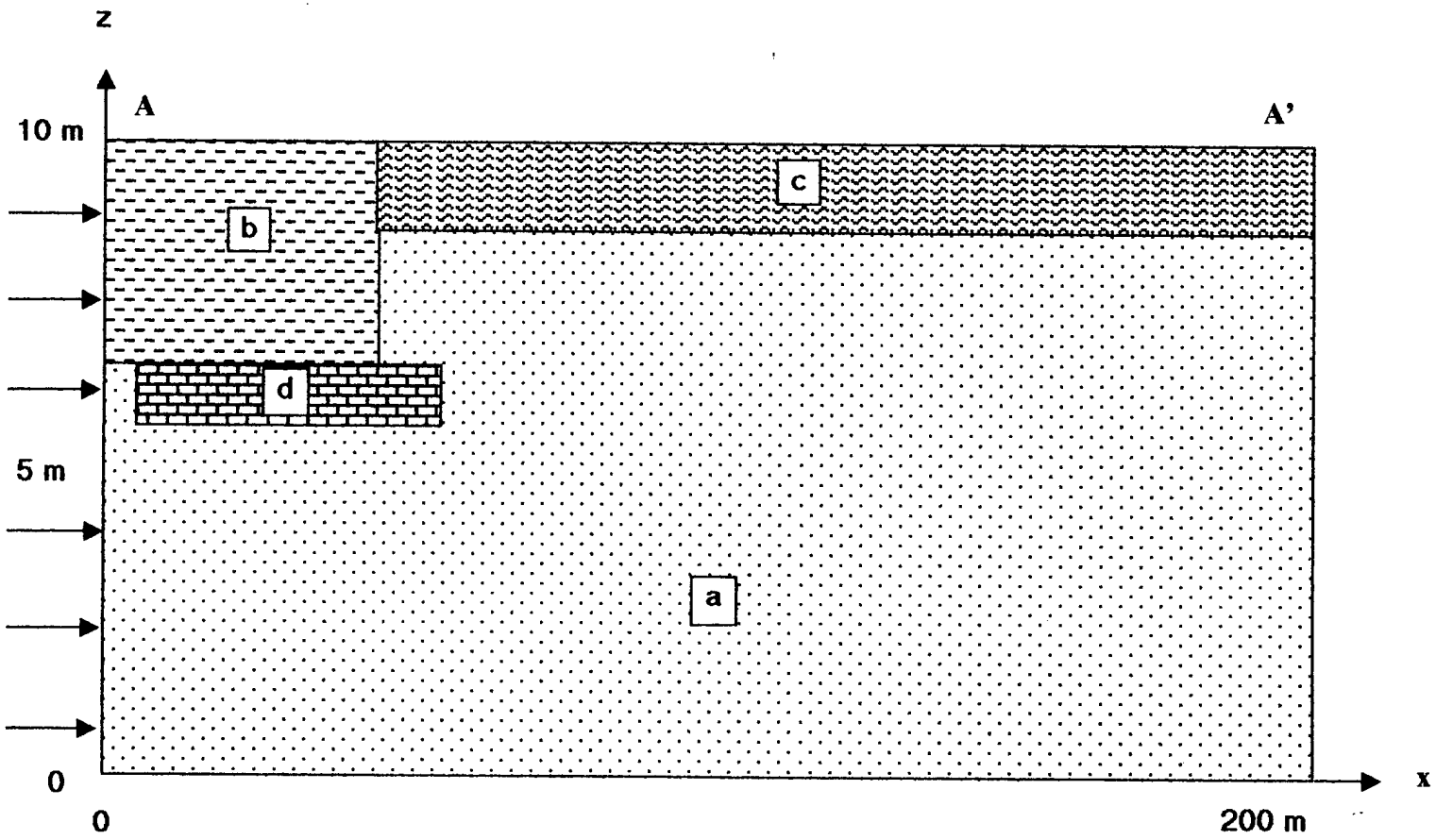

Figure 5: Vertical configuration of Trio Solvents aquifer from A to A' (not drawn to scale) with: a) the anaerobic aquifer region, b) the cottonwood root region, c) cattail root region, and d) the clay lens.

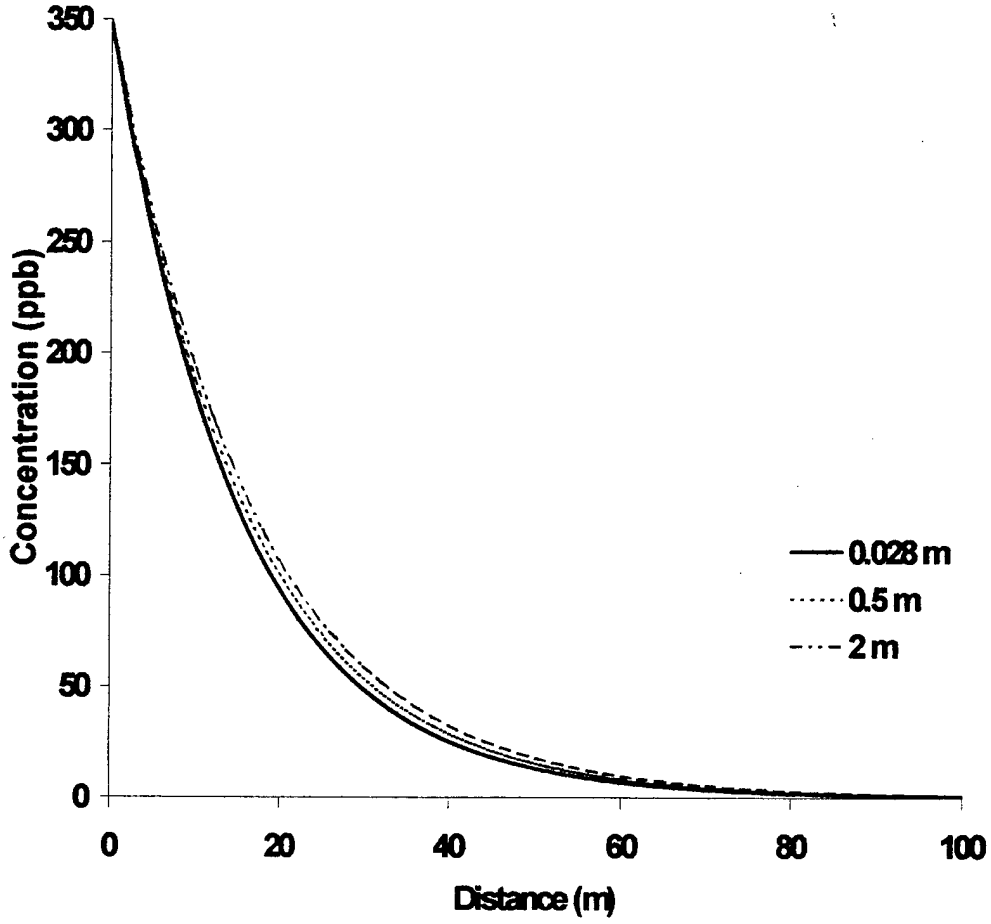

Figure 6: One-dimensional simulation results for segment-length comparisons. Results show TCE concentration profiles from A to 100 m downgradient for a simulation time of 6500 days.

stability. As a result of the smaller segment length and shorter time-step length, computation time increased. Results for 0.5 m (Pe = 83) and 2 m (Pe = 334) segment lengths, which allowed time-step length to be set at 1 day, took less than 1/600 of the computation time needed for the Pe = 5 simulation. The point where TCE concentrations dropped below the EPA's maximum contaminant level (MCL) of 5 ppb was 65, 68, and 72 m downgradient for the simulations with 0.028, 0.5, and 2.0 m segment lengths, respectively. This was interpreted to mean that the TCE plume would be degraded well before reaching Rush Lake, which was 250 m downgradient. Literature that addresses the evaluation of natural attenuation emphasizes the need for conservatism in model output (Brady et al., 1998; American Society for Testing and Materials, 1994). Therefore the time saved in calculation was considered to outweigh the additional numerical dispersion induced when using larger segment lengths.

Sensitivity analyses of the transport and degradation parameters were also completed to identify which parameters had the greatest influence on profile results. The 2 m segment, 6500 day simulation discussed above (parameter values in Table 3) was used as the reference profile for the sensitivity analyses. Rate parameters were varied by an order of magnitude from those used in the reference simulation. Variations of longitudinal dispersion (2.5 x 10-3 and 2.5 x 10-5 m2/d) and transverse dispersion (7.5 x 10-4 and 7.5 x 10-6 m2/d) gave no appreciable change from the concentration profile (data not shown), indicating that the system is advection-dominated. However, simulations in which the groundwater velocity (4.17 x 10-1 and 4.17 x 10-3 m/d) and degradation rates (0.0131 and 0.000131 d-1) were varied by a factor of 10 gave a large variance from the reference profile (Figure 7). As to be expected, simulations using a faster groundwater

Table 3: Transport and Degradation Parameters Used in Full 2-D Simulations

Δx	2 m
Δz	.667 m
Δt	1 d
v_x	0.0417 md^{-1}
Dx	2.5 x 10^{-4} m^2d^{-1}
Dz	7.5 x 10^{-5} m^2d^{-1}
K- aquifer	0.00131 d^{-1}
K- cottonwood	0.01 d^{-1}
K- cattail	0.0075 d^{-1}

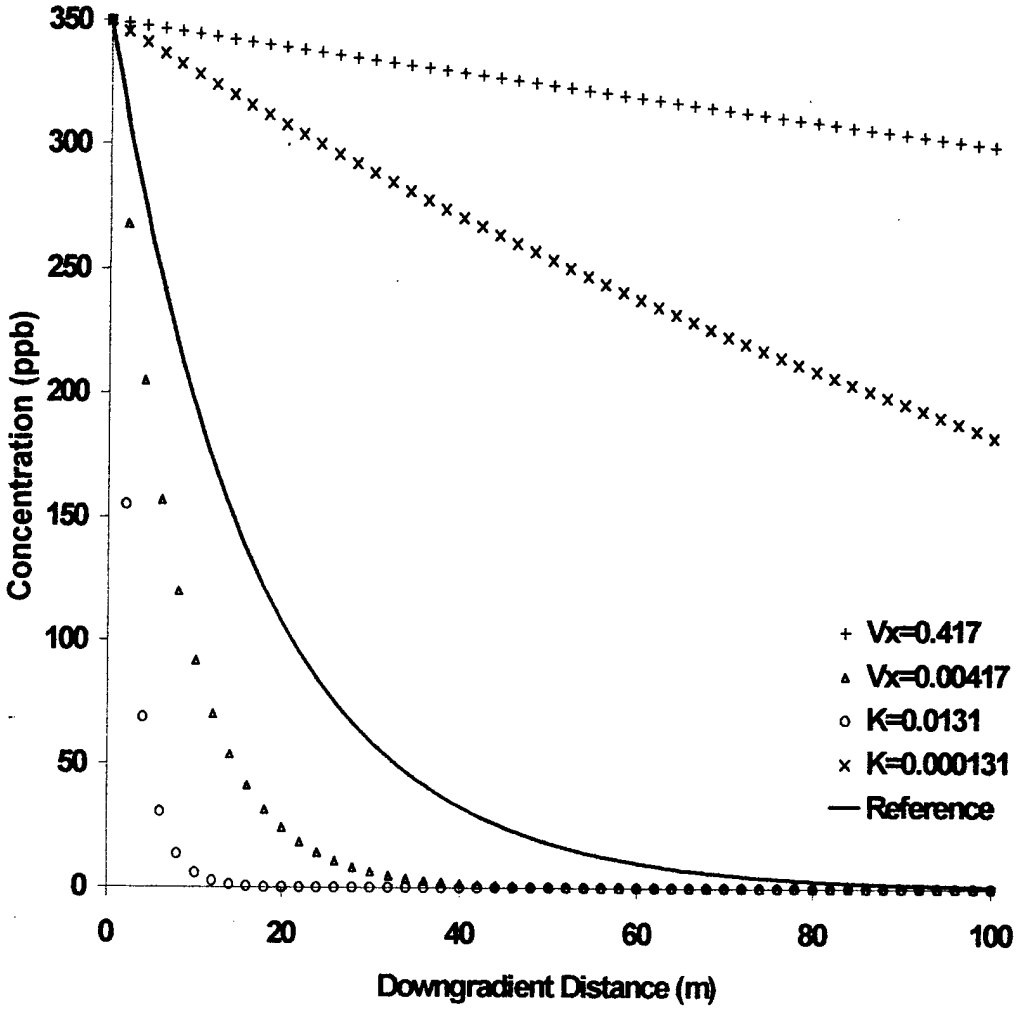

Figure 7: Sensitivity analyses results showing influence of varied groundwater velocity and degradation rates on the distance of plume migration.

velocity or a slower rate of degradation resulted in relatively higher TCE concentrations being propagated further downgradient while simulations with a slower groundwater velocity or a faster rate of degradation resulted in a reduction of the plume's travel distance.

A simulation for the vertical (x-z) plane from 0 to 10 m below surface and with the parameter values given in Table 3 was completed. This simulation included all three subsurface regions as well as the clay lens (Figure 5). Groundwater velocity and dispersion coefficients were assumed to be equal everywhere except in the clay lens that was assumed to be a no-flow zone with v_x, D_x, and D_z equal to zero. The source concentration of TCE was assumed to be a uniform 350 ppb at x = 0 along the z-axis. The model simulation was continued until the plume reached the point at which the natural attenuation equaled the mass flux of TCE (steady-state). This occurred after 6500 or more days for this simulation. Figure 8 gives the simulation results for the predicted TCE concentration in the vertical cross-section through the shallow aquifer shown in Figure 5. The TCE did not spread far downgradient in the shallow depths of the aquifer due to the higher degradation rates estimated for the cottonwood and cattail regions. The MCL of 5 ppb was reached at a distance of about 17 m downgradient of the source in the upper 4 to 5 m of the aquifer. In the deeper part of the aquifer, i.e. from 6 to 10 m, the MCL was reached approximately 72 m downgradient of the source.

The 2-D model presented and applied so far is for plumes that do not spread significantly in the horizontal direction. This is typically the case further downgradient from the source of pollution, especially in advection-dominated situations with low transverse dispersion. At the Trio Solvents site the field data indicated that the plume at

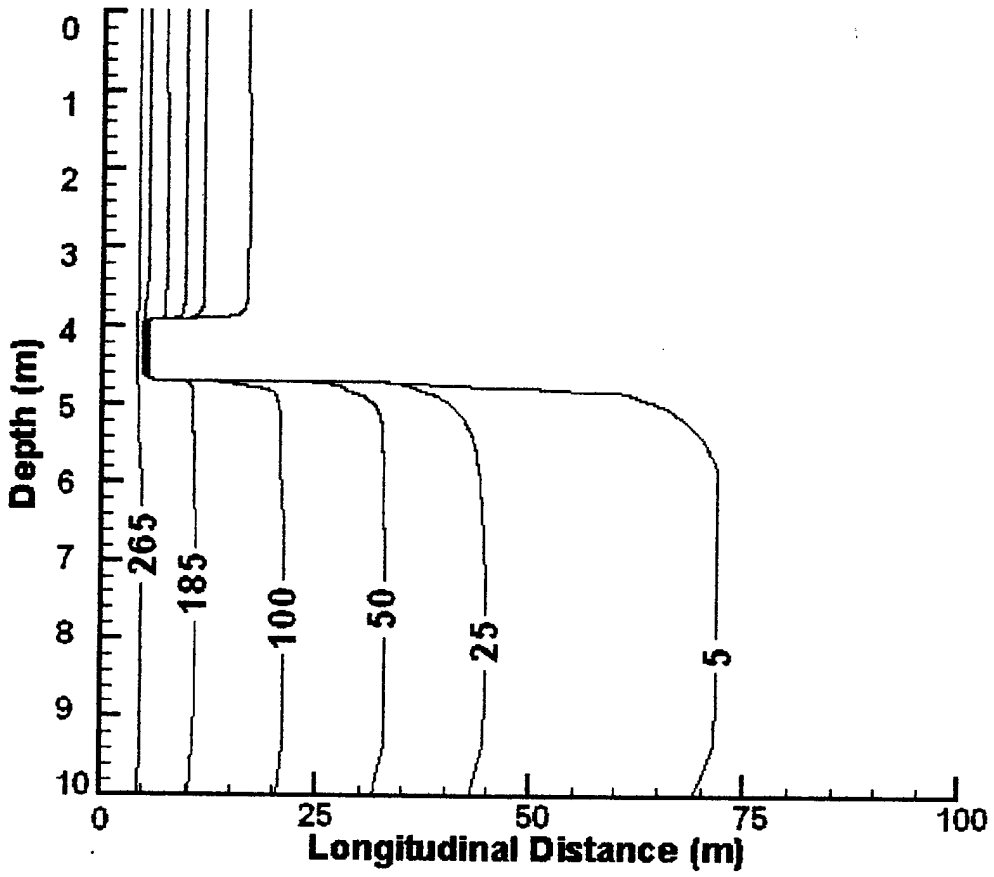

Figure 8: Modeling results of predicted TCE concentrations in vertical cross-section A-A' from Figure 3 for steady TCE input.

the starting point of the model domain (point A in Figure 3) was approximately 30 m wide. Upstream from point A and closer to the suspected TCE source area field observations indicate that the plume was as much as 60 m wide. For an aquifer thickness of 10 m these dimensions justify a 2-D approach for computations along the centerline of the plume.

However, near the lateral fringes of the plume TCE concentrations will naturally diminish. In order to obtain an approximate picture of the concentration field in a horizontal plane through the bottom part (10 m depth) of the aquifer, a simulation was made with the model after exchanging D_z and Δz for D_y and Δy. The coordinate y is in the horizontal transverse direction. The same numerical value was used for D_y and D_z. In this simulation the inflow concentrations to the horizontal model domain were specified as an approximate Gaussian distribution with a standard deviation of about 7.5 m and a maximum concentration of 350 ppb. The attenuation coefficient for the aquifer sediment at the 10 m depth (Table 3) was used for the simulation. Simulation results are shown in Figure 9.

Summary and Conclusions

A numerical spreadsheet-based model for a groundwater contaminant plume in a heterogeneous aquifer was developed and applied. The 2-D model incorporates advective and dispersive transport of a contaminant as well as contaminant removal by sorption and degradation. Heterogeneity in the aquifer and in these processes can be easily accounted for within the spreadsheets creating a very adaptable modeling tool for evaluating natural attenuation effects.

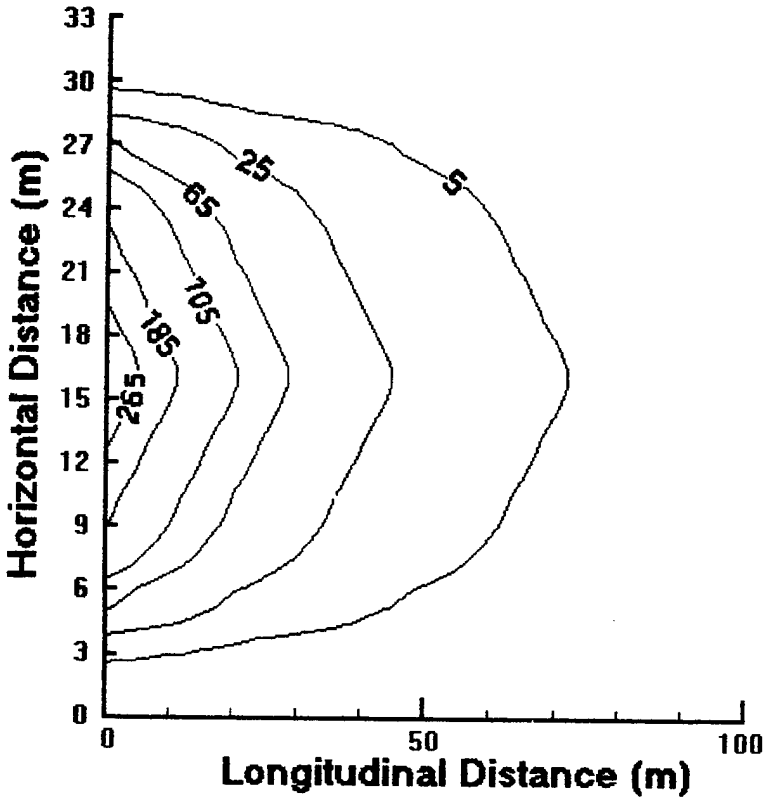

Figure 9: Modeling results of predicted TCE concentrations in horizontal cross-section at 10 m depth for steady TCE input.

The model output closely matched analytical solutions indicating that the governing equation for contaminant flow was solved correctly. However, when applying the model to a field site, results also reflect the accuracy of the input data. As the sensitivity analysis demonstrated, changes in flow velocity and degradation parameters of the advection-dominated domain alter model results significantly, whereas changes in dispersion coefficients did not. Application of the model to the Trio Solvents site with input parameters based on site knowledge and conservative estimates of attenuation rates indicated a high probability that natural processes will attenuate the TCE plume so that it will not impact Rush Lake. Known heterogeneity and multiple degradation regions were easily incorporated and model output showed which degradation regions had the greatest influence on plume reduction. Expansion of the model to three-dimensions and inclusion of additional attenuation processes such as volatilization could improve the applicability for future use.

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Appendix A

Instructions for Model Use

1. Determine desired segment length (Δx) and width (Δz) for discretization of the model domain and the time-step length (Δt).

2. Open desired Excel file containing the model program. Be sure to 'click' the "enable macro" option.

3. Enter the values for Δx, Δz, and Δt in the appropriate cells on the sheet labeled **Input**. The number of rows and columns needed for the model application will automatically be calculated below.

4. Copy cells A6 through C6 on the **Input** sheet down for the calculated number of rows, plus one more row. This extra row insures that the last row of the model domain still has a valid change in width value. This series of cells allows for incorporation of dispersion in the y-direction. Currently it is set so that the cells do not change in width as we move down gradient. However, if a value for dispersion in the y-direction is known and the width of the plume is known, spreading of the plume in the y-direction can be included in calculations.

5. Next, copy cell B6 on the remaining sheets (**Co, C, Po, P, Qo, Q, Ro, R, So, S, V, D_L, D_T, and k**) over and down for the desired number of columns and rows.

6. Establish boundary conditions. This is only necessary on the **Co** and **C** sheet. An upgradient source would be input by entering the source concentration values in row 5 for the desired columns. Zeros need not be entered around the flow domain to signify a no flux boundary, however if there are source areas along these boundaries, they should be added.

7. Enter initial conditions. This is done within the model domain on the **Co** sheet. Enter the known concentration values for each segment within the domain.

8. Enter transport and degradation parameters. Enter velocity (sheet **V**), longitudinal (sheet **DL**) and transverse (sheet **DT**) dispersion, and the first-order degradation rate (sheet **k**) parameters for each segment within the domain.

9. Press Ctrl+Shift+A to set the counter and to calculate the concentration values for the first time-step based on the initial conditions.

10. Creating the iteration loop: Highlight the concentration values from the model domain in sheet **C**, press Ctrl + C. Go to sheet **Co** and click on cell B6, from the Edit menu select Paste Special and select 'Paste Link.' This creates a loop where the next iteration uses the previous iteration's concentration values as initial conditions.

11. One iteration is equal to one time-step (Δt). In order to run the model for a desired number of iterations, go to the Tools menu, select Options and select the Calculation sheet. In the maximum iterations space enter the number of iterations. Click OK. Then press F9 to run the model simulation for the entered number of time-steps.

Appendix B

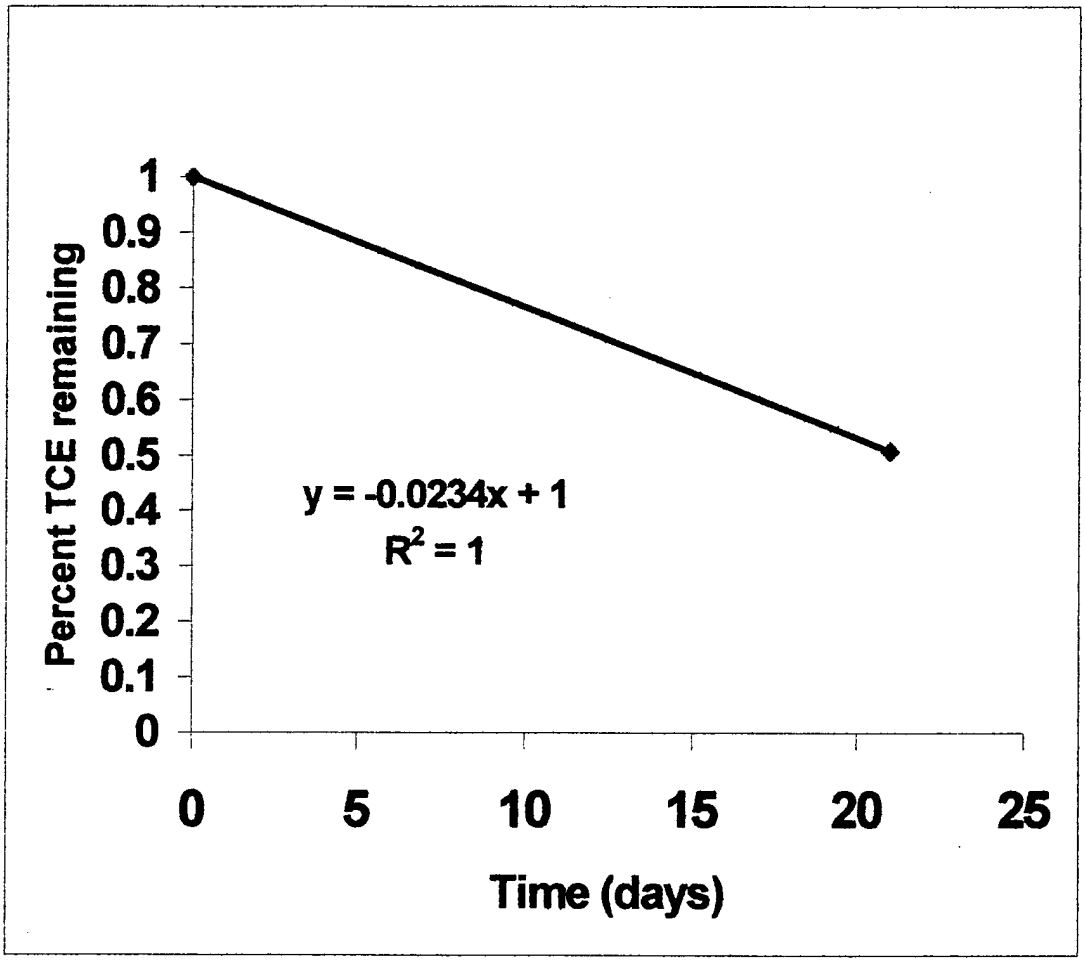

Figure B1: Calculation of first-order decay constant for TCE loss in cattail experiments. Data points are initial TCE present and TCE remaining in the microcosms at the end of the experiments conducted by Bankston et al (1999).

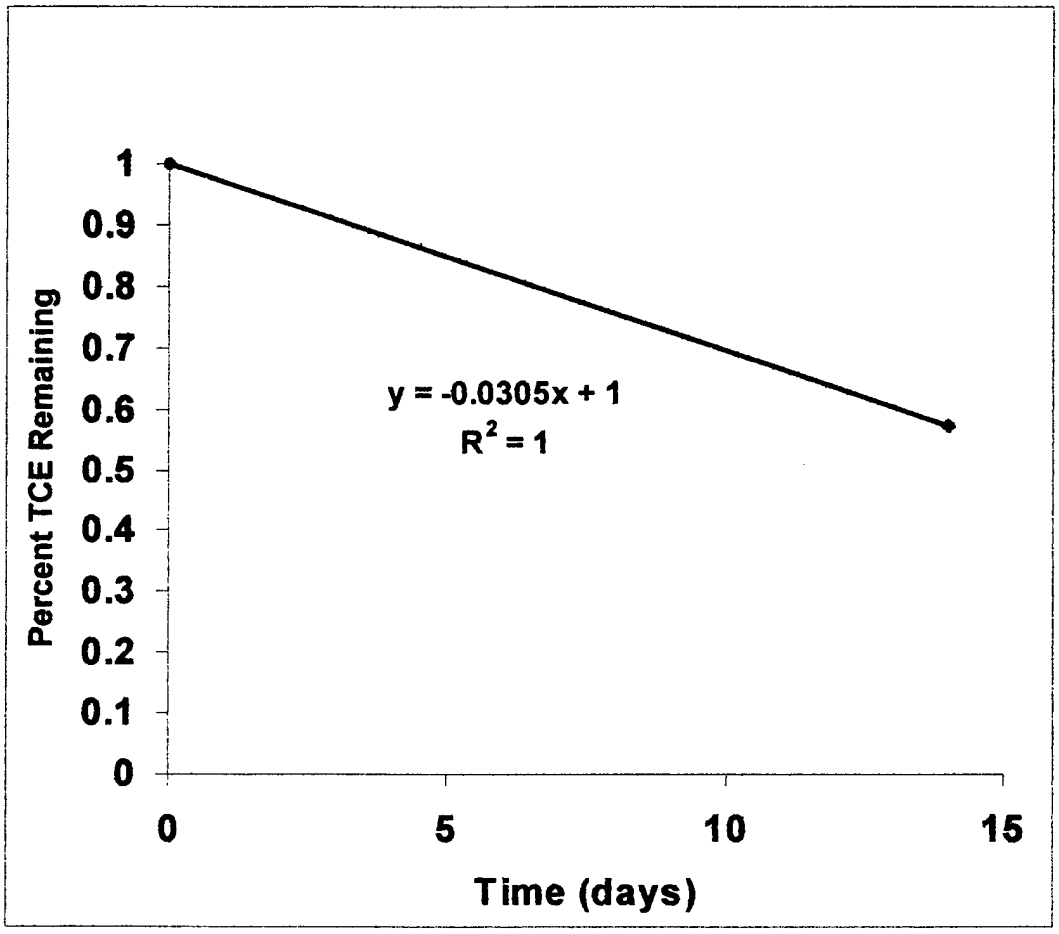

Figure B2: Calculation of first-order decay constant for TCE loss in cottonwood tree experiments. Data points are initial TCE present and TCE remaining in the microcosm at the end of the experiments conducted by Bankston et al (1999).

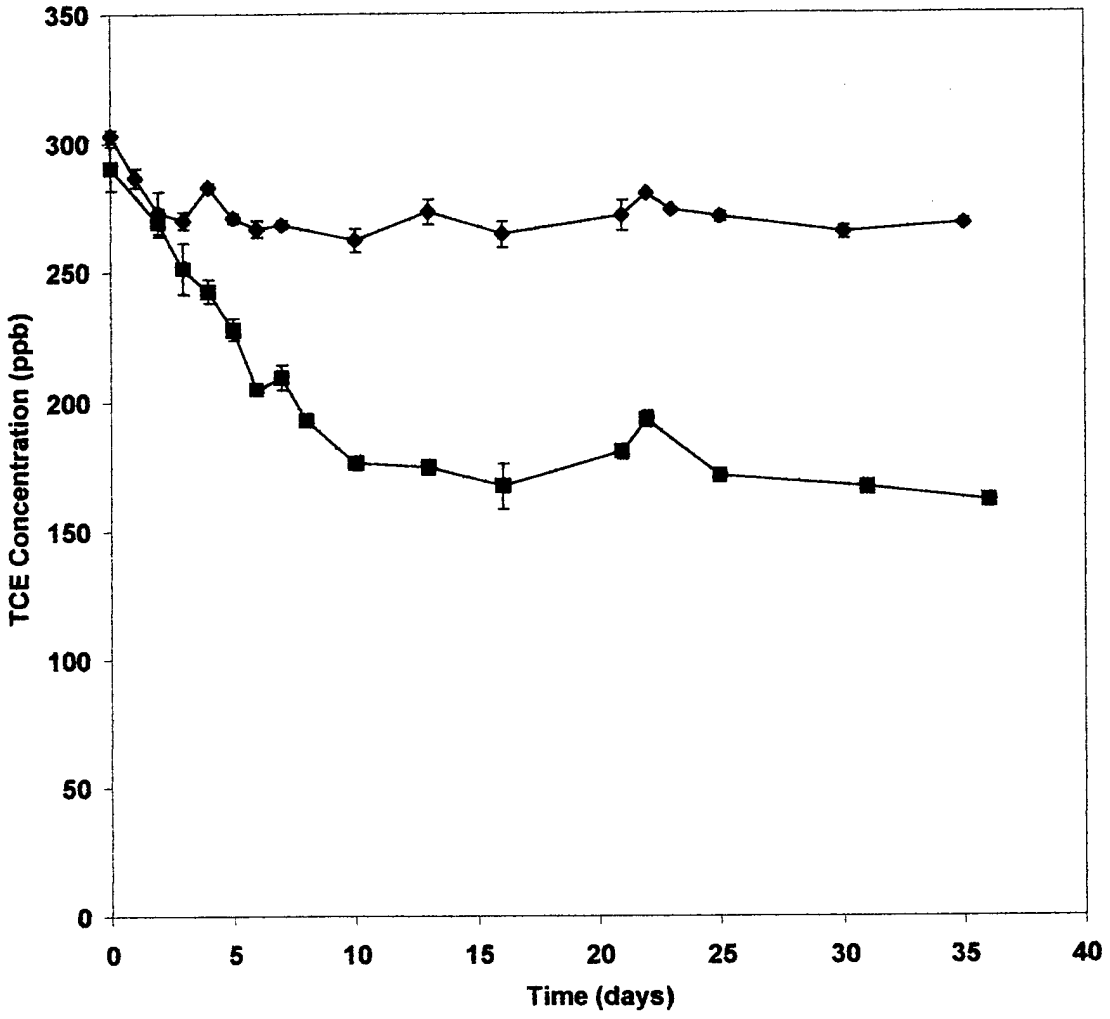

Figure B3: TCE loss in anaerobic aquifer sediment microcosms. Symbols are Experimental microcosms (■) and autoclaved control microcosms (◆). Soil for this experiment was collected from outside of the TCE plume at the Trio Solvents site (i.e. in clean sediment) at a depth of 8 m.

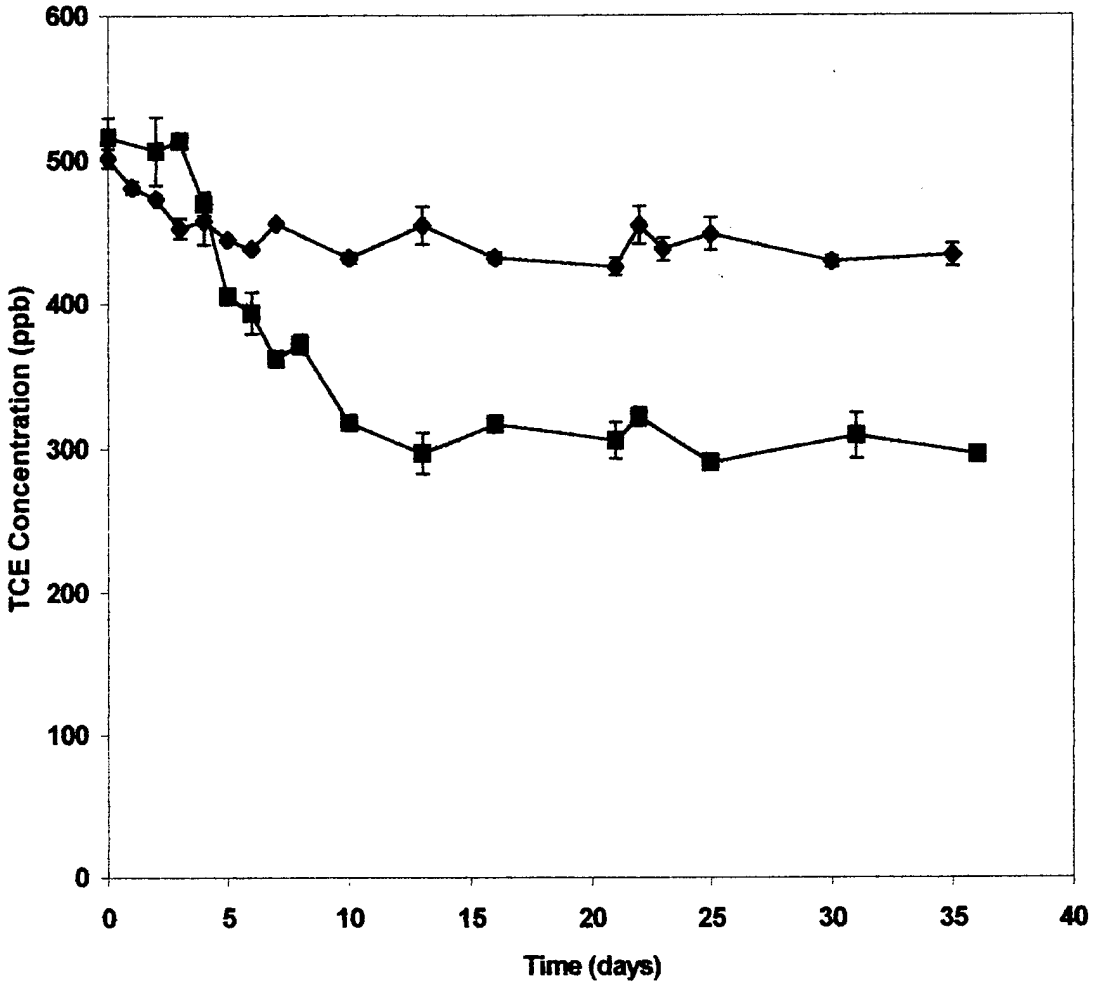

Figure B4: TCE loss in anaerobic aquifer sediment microcosms. Symbols are Experimental microcosms (■) and autoclaved control microcosms (◆). Soil for this experiment was collected from within the TCE plume at the Trio Solvents site (i.e. in contaminated sediment) at a depth of 8 m.

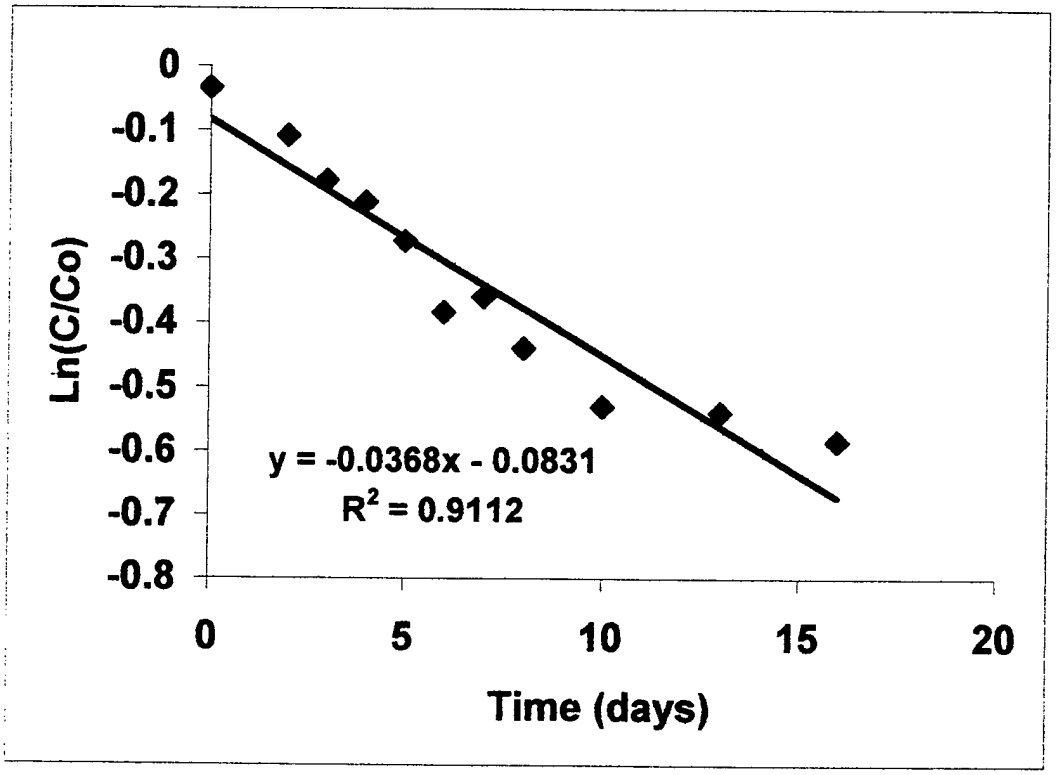

Figure B5: Calculation of first-order decay constant for TCE loss in "clean" aquifer sediment microcosms by trendline analysis. Only the data points collected during the first two weeks of the experiment were used for rate constant determination.

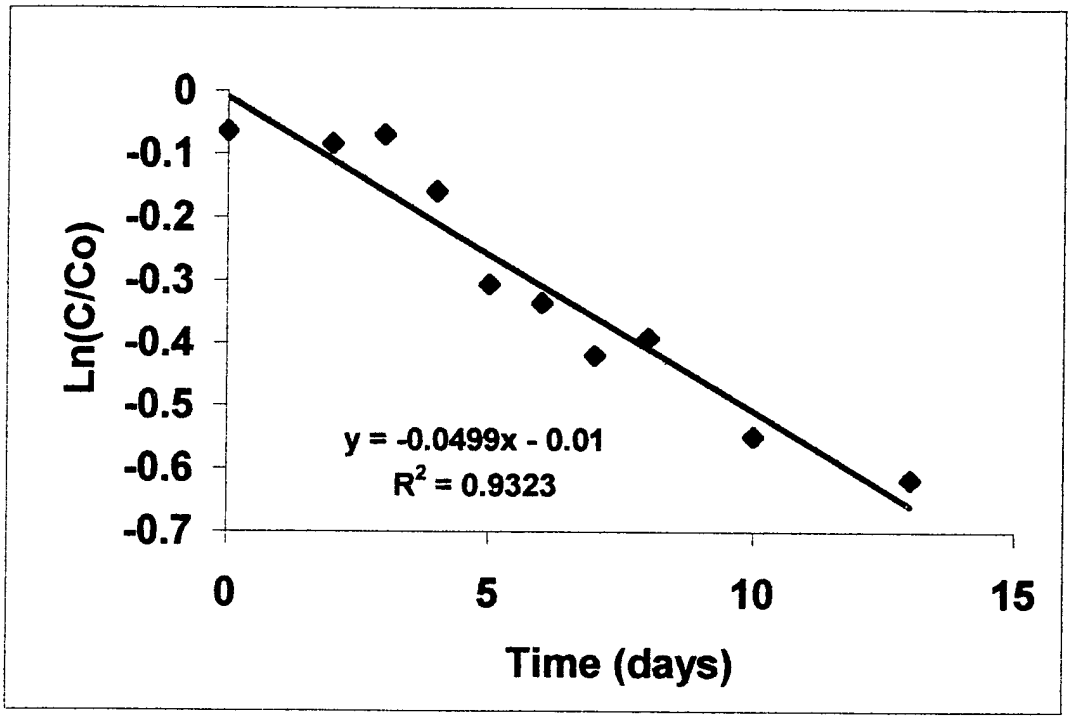

Figure B6: Calculation of first-order decay constant for TCE loss in "contaminated" aquifer sediment microcosms by trendline analysis. Only the data points collected during the first two weeks of the experiment were used for rate constant determination.

Appendix C

Table C1: Initial conditions for vertical cross-section model simulation

360	360	360	360	360	360	360	360	360	360	360	360	360	360	360
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table C2: Velocity Parameters for vertical cross-section model domain

0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417
0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417
0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0.0417	0	0

Table C3: Longitudinal dispersion parameters for vertical model domain

2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04
2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04
2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	2.50E-04	0	0

Table C4: Transverse dispersion parameters for vertical model domain

7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	0.00	0.00	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	0.00	0.00	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	0.00	0.00	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	0.00	0.00	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	0.00	0.00	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	0.00	0.00	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	0.00	0.00	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	0.00	0.00	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
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7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05
7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05	7.50E-05

Table C5: Degradation parameters for vertical model domain

0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131
0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131
0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0.00131	0	0	0.01	0.01	0.01	0.01

Table C6: Model output for 100 day simulation

350	350	350	350	350	350	350	350	350	350	350	350	350	350	350
215.5566	216.2816	216.2834	216.2834	216.2834	216.2834	216.2834	216.2834	216.2834	216.2834	216.2834	216.2834	216.2834	216.2816	215.5502
90.53981	90.98095	90.98218	90.98218	90.98218	90.98218	90.98218	90.98218	90.98212	90.96269	90.96268	90.97943	90.97948	90.97819	90.53047
27.64295	27.79782	27.79829	27.79829	27.79829	27.79829	27.79829	27.79821	27.7452	0	0	23.08131	23.11972	23.11937	22.98953
6.493929	6.532713	6.532832	6.532832	6.532832	6.532832	6.532832	6.532794	6.512757	0	0	4.818078	4.831423	4.831353	4.802187
1.224256	1.231791	1.231814	1.231814	1.231814	1.231814	1.231814	1.231804	1.227101	0	0	0.840134	0.843085	0.843073	0.83777
0.191018	0.192208	0.192212	0.192212	0.192212	0.192212	0.192212	0.19221	0.191378	0	0	0.124328	0.124827	0.124826	0.124022
0.025245	0.025403	0.025403	0.025403	0.025403	0.025403	0.025403	0.025403	0.025284	0	0	0.015843	0.015912	0.015911	0.015808
0.002877	0.002895	0.002895	0.002895	0.002895	0.002895	0.002895	0.002895	0.002881	0	0	0.00176	0.001768	0.001768	0.001757
0.000287	0.000289	0.000289	0.000289	0.000289	0.000289	0.000289	0.000289	0.000287	0	0	0.000172	0.000173	0.000173	0.000172
2.53E-05	2.54E-05	2.54E-05	2.54E-05	2.54E-05	2.54E-05	2.54E-05	2.54E-05	2.53E-05	0	0	1.61E-05	1.61E-05	1.61E-05	1.53E-05
1.99E-06	2E-06	2E-06	2E-06	2E-06	2E-06	2E-06	2E-06	1.99E-06	1.09E-09	8.21E-10	1.32E-06	1.33E-06	1.33E-06	1.21E-06
1.41E-07	1.42E-07	1.42E-07	1.42E-07	1.42E-07	1.42E-07	1.42E-07	1.42E-07	1.41E-07	1.39E-10	1.1E-10	9.76E-08	9.81E-08	9.81E-08	8.67E-08
9.09E-09	9.14E-09	9.14E-09	9.14E-09	9.14E-09	9.14E-09	9.14E-09	9.14E-09	9.09E-09	1.22E-11	9.96E-12	6.49E-09	6.52E-09	6.52E-09	5.62E-09
5.33E-10	5.36E-10	5.36E-10	5.36E-10	5.36E-10	5.36E-10	5.36E-10	5.36E-10	5.33E-10	8.7E-13	7.35E-13	3.91E-10	3.93E-10	3.93E-10	3.32E-10
2.87E-11	2.88E-11	2.88E-11	2.88E-11	2.88E-11	2.88E-11	2.88E-11	2.88E-11	2.87E-11	5.36E-14	4.67E-14	2.16E-11	2.17E-11	2.17E-11	1.8E-11
1.42E-12	1.43E-12	1.43E-12	1.43E-12	1.43E-12	1.43E-12	1.43E-12	1.43E-12	1.42E-12	2.93E-15	2.63E-15	1.09E-12	1.1E-12	1.1E-12	8.99E-13
6.5E-14	6.54E-14	6.54E-14	6.54E-14	6.54E-14	6.54E-14	6.54E-14	6.54E-14	6.5E-14	1.44E-16	1.33E-16	5.09E-14	5.11E-14	5.11E-14	4.15E-14
2.76E-15	2.78E-15	2.78E-15	2.78E-15	2.78E-15	2.78E-15	2.78E-15	2.78E-15	2.76E-15	6.49E-18	6.15E-18	2.2E-15	2.21E-15	2.21E-15	1.78E-15
1.09E-16	1.1E-16	1.1E-16	1.1E-16	1.1E-16	1.1E-16	1.1E-16	1.1E-16	1.09E-16	2.69E-19	2.61E-19	8.85E-17	8.89E-17	8.88E-17	7.08E-17
4.05E-18	4.07E-18	4.07E-18	4.07E-18	4.07E-18	4.07E-18	4.07E-18	4.07E-18	4.05E-18	1.03E-20	1.02E-20	3.32E-18	3.33E-18	3.33E-18	2.64E-18
1.4E-19	1.41E-19	1.41E-19	1.41E-19	1.41E-19	1.41E-19	1.41E-19	1.41E-19	1.4E-19	3.66E-22	3.72E-22	1.16E-19	1.17E-19	1.17E-19	9.2E-20
4.57E-21	4.59E-21	4.59E-21	4.59E-21	4.59E-21	4.59E-21	4.59E-21	4.59E-21	4.57E-21	1.22E-23	1.26E-23	3.83E-21	3.85E-21	3.85E-21	3.02E-21
1.4E-22	1.41E-22	1.41E-22	1.41E-22	1.41E-22	1.41E-22	1.41E-22	1.41E-22	1.4E-22	3.8E-25	4.02E-25	1.19E-22	1.19E-22	1.19E-22	9.31E-23
4.06E-24	4.08E-24	4.08E-24	4.08E-24	4.08E-24	4.08E-24	4.08E-24	4.08E-24	4.06E-24	1.11E-26	1.2E-26	3.47E-24	3.48E-24	3.48E-24	2.71E-24
1.11E-25	1.12E-25	1.12E-25	1.12E-25	1.12E-25	1.12E-25	1.12E-25	1.12E-25	1.11E-25	3.07E-28	3.38E-28	9.57E-26	9.61E-26	9.61E-26	7.46E-26
2.88E-27	2.9E-27	2.9E-27	2.9E-27	2.9E-27	2.9E-27	2.9E-27	2.9E-27	2.88E-27	8.02E-30	9E-30	2.5E-27	2.51E-27	2.51E-27	1.95E-27
7.11E-29	7.14E-29	7.14E-29	7.14E-29	7.14E-29	7.14E-29	7.14E-29	7.14E-29	7.1E-29	1.99E-31	2.27E-31	6.21E-29	6.24E-29	6.23E-29	4.82E-29
1.67E-30	1.67E-30	1.67E-30	1.67E-30	1.67E-30	1.67E-30	1.67E-30	1.67E-30	1.67E-30	4.67E-33	5.42E-33	1.47E-30	1.47E-30	1.47E-30	1.14E-30
3.72E-32	3.74E-32	3.74E-32	3.74E-32	3.74E-32	3.74E-32	3.74E-32	3.74E-32	3.72E-32	1.04E-34	1.23E-34	3.29E-32	3.31E-32	3.3E-32	2.55E-32
7.94E-34	7.97E-34	7.97E-34	7.97E-34	7.97E-34	7.97E-34	7.97E-34	7.97E-34	7.93E-34	2.22E-36	2.67E-36	7.06E-34	7.09E-34	7.08E-34	5.47E-34
1.62E-35	1.63E-35	1.63E-35	1.63E-35	1.63E-35	1.63E-35	1.63E-35	1.63E-35	1.62E-35	4.53E-38	5.53E-38	1.45E-35	1.45E-35	1.45E-35	1.12E-35
3.16E-37	3.17E-37	3.17E-37	3.17E-37	3.17E-37	3.17E-37	3.17E-37	3.17E-37	3.15E-37	8.81E-40	1.09E-39	2.84E-37	2.85E-37	2.84E-37	2.19E-37
5.91E-39	5.93E-39	5.93E-39	5.93E-39	5.93E-39	5.93E-39	5.93E-39	5.93E-39	5.9E-39	1.64E-41	2.07E-41	5.33E-39	5.35E-39	5.34E-39	4.12E-39
1.06E-40	1.06E-40	1.06E-40	1.06E-40	1.06E-40	1.06E-40	1.06E-40	1.06E-40	1.06E-40	2.94E-43	3.76E-43	9.6E-41	9.64E-41	9.63E-41	7.42E-41
1.83E-42	1.84E-42	1.84E-42	1.84E-42	1.84E-42	1.84E-42	1.84E-42	1.84E-42	1.83E-42	5.04E-45	6.56E-45	1.66E-42	1.67E-42	1.67E-42	1.28E-42
3.04E-44	3.05E-44	3.05E-44	3.05E-44	3.05E-44	3.05E-44	3.05E-44	3.05E-44	3.03E-44	8.33E-47	1.1E-46	2.77E-44	2.78E-44	2.78E-44	2.14E-44
4.86E-46	4.88E-46	4.88E-46	4.88E-46	4.88E-46	4.88E-46	4.88E-46	4.88E-46	4.85E-46	1.32E-48	1.77E-48	4.44E-46	4.46E-46	4.46E-46	3.43E-46
7.49E-48	7.52E-48	7.52E-48	7.52E-48	7.52E-48	7.52E-48	7.52E-48	7.52E-48	7.48E-48	2.03E-50	2.76E-50	6.87E-48	6.9E-48	6.89E-48	5.31E-48
1.11E-49	1.12E-49	1.12E-49	1.12E-49	1.12E-49	1.12E-49	1.12E-49	1.12E-49	1.11E-49	3E-52	4.14E-52	1.03E-49	1.03E-49	1.03E-49	7.93E-50
1.6E-51	1.61E-51	1.61E-51	1.61E-51	1.61E-51	1.61E-51	1.61E-51	1.61E-51	1.6E-51	4.29E-54	5.99E-54	1.48E-51	1.48E-51	1.48E-51	1.14E-51
2.23E-53	2.24E-53	2.24E-53	2.24E-53	2.24E-53	2.24E-53	2.24E-53	2.24E-53	2.22E-53	5.93E-56	8.39E-56	2.06E-53	2.07E-53	2.07E-53	1.59E-53
3E-55	3.01E-55	3.01E-55	3.01E-55	3.01E-55	3.01E-55	3.01E-55	3.01E-55	2.99E-55	7.93E-58	1.14E-57	2.78E-55	2.79E-55	2.79E-55	2.15E-55
3.91E-57	3.92E-57	3.92E-57	3.92E-57	3.92E-57	3.92E-57	3.92E-57	3.92E-57	3.9E-57	1.03E-59	1.49E-59	3.63E-57	3.65E-57	3.64E-57	2.81E-57
4.94E-59	4.96E-59	4.96E-59	4.96E-59	4.96E-59	4.96E-59	4.96E-59	4.96E-59	4.93E-59	1.29E-61	1.9E-61	4.6E-59	4.62E-59	4.62E-59	3.56E-59
6.06E-61	6.08E-61	6.08E-61	6.08E-61	6.08E-61	6.08E-61	6.08E-61	6.08E-61	6.05E-61	1.57E-63	2.34E-63	5.66E-61	5.68E-61	5.67E-61	4.38E-61
7.22E-63	7.24E-63	7.24E-63	7.24E-63	7.24E-63	7.24E-63	7.24E-63	7.24E-63	7.2E-63	1.86E-65	2.8E-65	6.75E-63	6.77E-63	6.77E-63	5.23E-63
8.35E-65	8.38E-65	8.38E-65	8.38E-65	8.38E-65	8.38E-65	8.38E-65	8.38E-65	8.33E-65	2.13E-67	3.25E-67	7.82E-65	7.85E-65	7.84E-65	6.06E-65
9.39E-67	9.42E-67	9.42E-67	9.42E-67	9.42E-67	9.42E-67	9.42E-67	9.42E-67	9.38E-67	2.38E-69	3.68E-69	8.82E-67	8.84E-67	8.84E-67	6.83E-67
1.03E-68	1.03E-68	1.03E-68	1.03E-68	1.03E-68	1.03E-68	1.03E-68	1.03E-68	1.03E-68	2.59E-71	4.04E-71	9.67E-69	9.7E-69	9.69E-69	7.49E-69
1.1E-70	1.1E-70	1.1E-70	1.1E-70	1.1E-70	1.1E-70	1.1E-70	1.1E-70	1.09E-70	2.74E-73	4.32E-73	1.03E-70	1.03E-70	1.03E-70	8E-71
1.14E-72	1.14E-72	1.14E-72	1.14E-72	1.14E-72	1.14E-72	1.14E-72	1.14E-72	1.13E-72	2.82E-75	4.51E-75	1.07E-72	1.08E-72	1.07E-72	8.32E-73

Table C7: Model output for 2000 day simulation

350	350	350	350	350	350	350	350	350	350	350	350	350	350	350
308.7399	310.9248	310.9403	310.9405	310.9405	310.9405	310.9405	310.9405	310.9404	310.9388	310.9387	310.9397	310.9396	310.9241	308.7392
272.3574	276.1987	276.2395	276.2399	276.2399	276.2399	276.2399	276.2398	276.2308	275.5929	275.591	275.9584	275.9621	275.9215	272.0888
240.2743	245.3394	245.411	245.4119	245.4119	245.4119	245.4118	245.3994	243.6671	0	0	140.3752	140.9507	140.9223	138.4148
211.9809	217.9179	218.0227	218.0242	218.0242	218.0242	218.0239	217.9915	214.9529	0	0	71.40764	71.99093	71.97253	70.41442
187.0283	193.5526	193.6905	193.6928	193.6928	193.6928	193.6922	193.6355	189.6318	0	0	36.32503	36.76894	36.75761	35.82183
165.0205	171.9036	172.0731	172.0763	172.0764	172.0764	172.0752	171.9923	167.3013	0	0	18.47883	18.77921	18.77245	18.22389
145.6081	152.668	152.8665	152.8707	152.8708	152.8708	152.869	152.7599	147.6063	0	0	9.400485	9.591057	9.587123	9.271313
128.4817	135.575	135.799	135.8043	135.8044	135.8043	135.8018	135.6678	130.2323	0	0	4.782261	4.89834	4.896088	4.716812
113.366	120.3803	120.626	120.6324	120.6325	120.6324	120.6291	120.4724	114.8994	0	0	2.434276	2.503078	2.501795	2.4
100.0133	106.8612	107.1245	107.1319	107.1321	107.132	107.1279	106.9513	101.3559	0	0	2.147734	2.223145	2.216724	1.393871
88.19821	94.81138	95.088	95.09639	95.09659	95.09649	95.09153	94.89836	89.37734	0.631553	0.017875	1.895122	1.974358	1.961164	0.812667
77.71286	84.03673	84.32216	84.33143	84.33167	84.33155	84.3258	84.11978	78.75068	1.106994	0.035258	1.67238	1.753214	1.733338	0.476553
68.36457	74.35385	74.64339	74.6534	74.65367	74.65353	74.64707	74.43229	69.27888	1.451321	0.051376	1.475868	1.556541	1.530879	0.281845
59.97642	65.59167	65.88038	65.89093	65.89123	65.89106	65.88403	65.66488	60.78128	1.684131	0.065606	1.302273	1.381409	1.351165	0.16876
52.39114	57.59669	57.87943	57.89028	57.89061	57.89041	57.88298	57.66413	53.09747	1.820734	0.077423	1.148522	1.225043	1.191486	0.102818
45.47709	50.24078	50.51238	50.52326	50.5236	50.52339	50.51575	50.30198	46.09335	1.873536	0.086384	1.011723	1.084777	1.049126	0.06413
39.13448	43.4291	43.68456	43.69519	43.69553	43.69531	43.68769	43.48369	39.66745	1.853552	0.092151	0.889161	0.958052	0.921442	0.041215
33.29923	37.10509	37.33998	37.35007	37.3504	37.35018	37.3428	37.15286	33.7547	1.771777	0.094534	0.778356	0.842497	0.805968	0.027443
27.9422	31.25027	31.46102	31.47033	31.47064	31.47043	31.46351	31.29118	28.32566	1.640128	0.093545	0.677183	0.73607	0.700568	0.018982
23.06311	25.87755	26.0618	26.07013	26.07041	26.07022	26.06393	25.91178	23.38028	1.471731	0.089427	0.584005	0.637216	0.603584	0.013618
18.67988	21.01931	21.17607	21.1833	21.18355	21.18338	21.17784	21.04725	18.93697	1.280525	0.082653	0.497778	0.544999	0.513951	0.010073
14.81571	16.71268	16.84234	16.84842	16.84864	16.84849	16.84377	16.73491	15.01952	1.080324	0.073885	0.418073	0.459132	0.431224	0.007613
11.48683	12.98551	13.08968	13.09464	13.09482	13.09469	13.0908	13.00271	11.64458	0.883662	0.063893	0.344984	0.379888	0.35549	0.005819
8.69343	9.845942	9.927212	9.931129	9.93127	9.931168	9.928061	9.858892	8.812498	0.700737	0.053459	0.278951	0.307901	0.287177	0.004454
6.41534	7.277477	7.339019	7.342016	7.342125	7.342045	7.339645	7.286955	6.502887	0.538718	0.043286	0.22052	0.24391	0.226822	0.003386
4.61249	5.239558	5.284788	5.287011	5.287092	5.287032	5.285236	5.246299	4.675157	0.401557	0.033925	0.170117	0.1885	0.174832	0.00254
3.229222	3.672581	3.704846	3.706444	3.706503	3.706459	3.705157	3.677241	3.272873	0.290265	0.025745	0.127877	0.141917	0.131318	0.001872
2.200688	2.505385	2.527729	2.528843	2.528884	2.528853	2.527938	2.508515	2.230269	0.203526	0.018924	0.093564	0.103979	0.096011	0.00135
1.459637	1.66319	1.678214	1.678968	1.678996	1.678974	1.678351	1.665234	1.479139	0.138475	0.013479	0.066585	0.074085	0.068279	0.00095
0.942207	1.074413	1.084226	1.084721	1.084739	1.084725	1.084313	1.07571	0.954714	0.091458	0.009308	0.046067	0.051309	0.047208	0.000652
0.59197	0.675473	0.681701	0.682016	0.682028	0.682019	0.681755	0.676274	0.599776	0.058662	0.006234	0.030977	0.034533	0.031724	0.000436
0.362061	0.413366	0.417208	0.417403	0.417411	0.417405	0.41724	0.413847	0.366802	0.036558	0.004052	0.020244	0.022586	0.020721	0.000283
0.215625	0.246298	0.248604	0.248722	0.248726	0.248722	0.248623	0.24658	0.218428	0.022147	0.002557	0.012859	0.014357	0.013155	0.000179
0.125077	0.14293	0.144276	0.144344	0.144347	0.144345	0.144286	0.14309	0.126691	0.013048	0.001568	0.007941	0.008871	0.008119	0.00011
0.070691	0.08081	0.081575	0.081614	0.081616	0.081614	0.081581	0.080899	0.071596	0.007481	0.000934	0.004769	0.00533	0.004873	6.61E-05
0.038941	0.04453	0.044953	0.044975	0.044976	0.044975	0.044956	0.044577	0.039436	0.004175	0.000541	0.002786	0.003115	0.002845	3.85E-05
0.020916	0.023924	0.024153	0.024165	0.024165	0.024165	0.024154	0.02395	0.02118	0.00227	0.000305	0.001584	0.001772	0.001617	2.19E-05
0.010959	0.012538	0.012658	0.012664	0.012664	0.012664	0.012659	0.012551	0.011096	0.001203	0.000168	0.000876	0.000981	0.000894	1.21E-05
0.005603	0.006411	0.006473	0.006476	0.006476	0.006476	0.006473	0.006418	0.005672	0.000621	8.96E-05	0.000472	0.000529	0.000482	6.5E-06
0.002796	0.0032	0.003231	0.003233	0.003233	0.003233	0.003231	0.003204	0.002831	0.000313	4.67E-05	0.000248	0.000278	0.000253	3.41E-06
0.001363	0.00156	0.001575	0.001576	0.001576	0.001576	0.001575	0.001562	0.00138	0.000154	2.37E-05	0.000127	0.000142	0.00013	1.74E-06
0.000649	0.000743	0.00075	0.000751	0.000751	0.000751	0.00075	0.000744	0.000657	7.39E-05	1.18E-05	6.35E-05	7.11E-05	6.47E-05	8.7E-07
0.000302	0.000346	0.000349	0.000349	0.000349	0.000349	0.000349	0.000346	0.000306	3.47E-05	5.7E-06	3.09E-05	3.47E-05	3.15E-05	4.24E-07
0.000138	0.000157	0.000159	0.000159	0.000159	0.000159	0.000159	0.000158	0.000139	1.59E-05	2.69E-06	1.47E-05	1.65E-05	1.5E-05	2.01E-07
6.12E-05	7.01E-05	7.08E-05	7.08E-05	7.08E-05	7.08E-05	7.08E-05	7.02E-05	6.19E-05	7.13E-06	1.24E-06	6.84E-06	7.67E-06	6.96E-06	9.35E-08
2.67E-05	3.05E-05	3.08E-05	3.08E-05	3.08E-05	3.08E-05	3.08E-05	3.06E-05	2.7E-05	3.12E-06	5.6E-07	3.11E-06	3.48E-06	3.16E-06	4.24E-08
1.14E-05	1.3E-05	1.31E-05	1.32E-05	1.32E-05	1.32E-05	1.31E-05	1.3E-05	1.15E-05	1.34E-06	2.47E-07	1.38E-06	1.55E-06	1.4E-06	1.88E-08
4.75E-06	5.44E-06	5.49E-06	5.49E-06	5.49E-06	5.49E-06	5.49E-06	5.44E-06	4.8E-06	5.63E-07	1.07E-07	5.98E-07	6.71E-07	6.08E-07	8.16E-09
1.94E-06	2.22E-06	2.24E-06	2.25E-06	2.25E-06	2.25E-06	2.25E-06	2.23E-06	1.96E-06	2.31E-07	4.5E-08	2.54E-07	2.85E-07	2.58E-07	3.46E-09
7.78E-07	8.91E-07	9E-07	9E-07	9E-07	9E-07	9E-07	8.92E-07	7.87E-07	9.32E-08	1.86E-08	1.06E-07	1.18E-07	1.07E-07	1.44E-09
3.06E-07	3.5E-07	3.53E-07	3.53E-07	3.53E-07	3.53E-07	3.53E-07	3.5E-07	3.09E-07	3.68E-08	7.53E-09	4.29E-08	4.82E-08	4.36E-08	5.85E-10

Table C8: Model output for 6500 day simulation

350	350	350	350	350	350	350	350	350	350	350	350	350	350	350
308.7399	310.9248	310.9403	310.9405	310.9405	310.9405	310.9405	310.9405	310.9404	310.9388	310.9387	310.9397	310.9396	310.9241	308.7392
272.3574	276.1987	276.2395	276.2399	276.2399	276.2399	276.2399	276.2398	276.2308	275.5929	275.591	275.9584	275.9621	275.9215	272.0888
240.2743	245.3394	245.411	245.4119	245.4119	245.4119	245.4118	245.3994	243.6671	0	0	140.3752	140.9507	140.9223	138.4148
211.9809	217.918	218.0227	218.0242	218.0242	218.0242	218.0239	217.9916	214.9529	0	0	71.40764	71.99093	71.97253	70.41442
187.0284	193.5527	193.6907	193.693	193.693	193.693	193.6923	193.6356	189.632	0	0	36.32503	36.76894	36.75761	35.82183
165.0211	171.9043	172.0739	172.0771	172.0771	172.0771	172.0759	171.993	167.302	0	0	18.47883	18.77921	18.77246	18.22389
145.6104	152.6707	152.8693	152.8735	152.8735	152.8735	152.8717	152.7626	147.6087	0	0	9.400485	9.591058	9.587124	9.271314
128.4891	135.5835	135.8077	135.8129	135.813	135.813	135.8105	135.6764	130.2399	0	0	4.782261	4.89834	4.896089	4.716813
113.3863	120.404	120.65	120.6564	120.6565	120.6564	120.6531	120.4962	114.9204	0	0	2.434277	2.503079	2.501795	2.400001
100.0635	106.9197	107.1838	107.1912	107.1914	107.1913	107.1871	107.01	101.4077	0	0	2.147739	2.223151	2.21673	1.393872
88.31019	94.94199	95.22026	95.22875	95.22896	95.22885	95.22383	95.02949	89.49264	0.633434	0.017904	1.895148	1.974386	1.961191	0.812669
77.94107	84.30299	84.5918	84.60128	84.60153	84.6014	84.59552	84.38703	78.98517	1.113978	0.035409	1.672481	1.753324	1.733442	0.476556
68.79264	74.85349	75.14941	75.15981	75.1601	75.15994	75.15324	74.93368	69.71806	1.469389	0.051865	1.47619	1.556891	1.531207	0.281852
60.7208	66.46088	66.76076	66.772	66.77233	66.77214	66.76465	66.53696	61.54405	1.72293	0.066846	1.303143	1.382358	1.352049	0.168775
53.59851	59.00726	59.30827	59.32024	59.32062	59.3204	59.31219	59.07912	54.33346	1.894054	0.080097	1.150581	1.227295	1.193574	0.102851
47.31378	52.38785	52.68749	52.70009	52.70051	52.70026	52.6914	52.45548	47.97209	1.998994	0.091493	1.016069	1.089545	1.053529	0.064195
41.76783	46.50952	46.8056	46.81874	46.8192	46.81891	46.80947	46.57296	42.35937	2.05125	0.101004	0.89746	0.967184	0.929846	0.041335
36.8736	41.2895	41.58016	41.59374	41.59423	41.59391	41.58398	41.34886	37.40671	2.062024	0.108669	0.792865	0.858505	0.820656	0.027648
32.5543	36.65425	36.93794	36.95183	36.95236	36.95201	36.94167	36.70968	33.03604	2.040573	0.114577	0.700616	0.761985	0.724282	0.01931
28.74221	32.5384	32.81383	32.82796	32.82852	32.82814	32.81747	32.59006	29.17862	1.994518	0.11885	0.619246	0.676273	0.639231	0.014107
25.37762	28.8839	29.15004	29.1643	29.16489	29.16449	29.15357	28.93197	25.77384	1.930106	0.121627	0.547461	0.600165	0.56418	0.010758
22.40785	25.63913	25.8952	25.90951	25.91012	25.90969	25.89861	25.68381	22.7683	1.852434	0.123062	0.484121	0.532591	0.497953	0.008519
19.78646	22.75827	23.00367	23.01794	23.01858	23.01813	23.00695	22.79975	20.11494	1.765632	0.123308	0.428224	0.472598	0.439515	0.006957
17.47248	20.20057	20.43491	20.44907	20.44972	20.44926	20.43806	20.23904	17.77228	1.673024	0.122519	0.378885	0.419341	0.387948	0.005816
15.42976	17.92987	18.1529	18.16689	18.16755	18.16707	18.15591	17.96552	15.70375	1.577266	0.120842	0.335326	0.372067	0.342443	0.004947
13.62642	15.91401	16.12564	16.13939	16.14007	16.13957	16.12851	15.94704	13.87711	1.480454	0.118416	0.296862	0.330106	0.302287	0.004259
12.03435	14.12446	14.3247	14.33816	14.33885	14.33834	14.32743	14.15503	12.26392	1.384226	0.115369	0.262889	0.292865	0.26685	0.003697
10.62873	12.53586	12.72482	12.73795	12.73864	12.73813	12.72741	12.56413	10.83912	1.289839	0.11182	0.232876	0.259814	0.235576	0.003228
9.387661	11.12567	11.30356	11.31633	11.31702	11.3165	11.30602	11.15182	9.580593	1.198239	0.107876	0.206353	0.230484	0.207975	0.002829
8.291845	9.873902	10.04099	10.05336	10.05405	10.05352	10.04331	9.898074	8.468848	1.110115	0.103632	0.18291	0.204458	0.183615	0.002485
7.324236	8.762785	8.919386	8.931334	8.932019	8.931495	8.921581	8.78512	7.486679	1.025951	0.099172	0.162183	0.181365	0.162114	0.002187
6.469799	7.77654	7.923025	7.934531	7.935208	7.934686	7.925095	7.797172	6.618912	0.946065	0.094571	0.143852	0.160875	0.143136	0.001927
5.715264	6.901157	7.037923	7.048973	7.049641	7.049123	7.039872	6.920209	5.852158	0.87064	0.089893	0.127636	0.142697	0.126384	0.001699
5.048924	6.124192	6.251661	6.262246	6.262902	6.26239	6.253493	6.141782	5.174604	0.799752	0.085193	0.113286	0.126569	0.111597	0.001499
4.460444	5.434599	5.553205	5.563319	5.563962	5.563458	5.554925	5.450833	4.575824	0.733396	0.080516	0.100583	0.112262	0.098543	0.001323
3.940707	4.822565	4.932752	4.942395	4.943023	4.942528	4.934366	4.837544	4.046618	0.671502	0.075903	0.089335	0.09957	0.08702	0.001168
3.481663	4.27938	4.381596	4.390769	4.39138	4.390896	4.383108	4.293198	3.578865	0.613952	0.071385	0.079372	0.088312	0.076847	0.001031
3.076208	3.79731	3.891998	3.900706	3.9013	3.900827	3.893413	3.810053	3.165398	0.56059	0.066987	0.070545	0.078325	0.067865	0.00091
2.718072	3.369487	3.457086	3.465337	3.465912	3.465453	3.45841	3.381236	2.799888	0.511238	0.062731	0.062721	0.069467	0.059935	0.000804
2.401719	2.989816	3.070754	3.078558	3.079113	3.078668	3.071991	3.000646	2.476749	0.465698	0.058632	0.055784	0.061611	0.052934	0.00071
2.122265	2.652882	2.727578	2.734945	2.735481	2.735049	2.728733	2.662863	2.191047	0.423764	0.054702	0.049631	0.054643	0.046752	0.000627
1.875394	2.353883	2.422738	2.429681	2.430197	2.42978	2.423815	2.363077	1.938427	0.385222	0.050948	0.044171	0.048462	0.041294	0.000553
1.657301	2.08855	2.151954	2.158487	2.158982	2.158581	2.152958	2.097019	1.715042	0.349859	0.047376	0.039326	0.042981	0.036474	0.000489
1.464621	1.853097	1.911421	1.917559	1.918033	1.917647	1.912356	1.860895	1.517495	0.317466	0.043988	0.035024	0.03812	0.032218	0.000432
1.294387	1.644163	1.69776	1.703518	1.703972	1.703602	1.69863	1.651341	1.342783	0.287835	0.040783	0.031203	0.033808	0.028459	0.000381
1.143978	1.458763	1.50797	1.513364	1.513797	1.513443	1.508779	1.465369	1.188256	0.260768	0.037761	0.027808	0.029985	0.02514	0.000337
1.011078	1.294246	1.339382	1.344428	1.344841	1.344503	1.340134	1.300323	1.051571	0.236074	0.034918	0.02479	0.026594	0.022208	0.000298
0.893643	1.148261	1.189626	1.194341	1.194734	1.194412	1.190325	1.153851	0.930658	0.213569	0.032249	0.022107	0.023587	0.019619	0.000263
0.789868	1.018719	1.056596	1.060996	1.061369	1.061063	1.057245	1.023858	0.823687	0.193082	0.029749	0.01972	0.02092	0.017333	0.000232
0.698153	0.90376	0.938415	0.942516	0.942869	0.942578	0.939017	0.908483	0.729038	0.174449	0.027412	0.017596	0.018555	0.015313	0.000205
0.615659	0.799867	0.831469	0.835277	0.83561	0.835335	0.832026	0.804195	0.643781	0.157135	0.025167	0.015668	0.016419	0.013498	0.000181

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